

The Mott-Hubbard transition and the paramagnetic insulating state in the two-dimensional Hubbard model

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Abstract. – The Mott-Hubbard transition is studied in the context of the two-dimensional Hubbard model. Analytical calculations show the existence of a critical value U_c of the potential strength which separates a paramagnetic metallic phase from a paramagnetic insulating phase. Calculations of the density of states and double occupancy show that the ground state in the insulating phase contains always a small fraction of empty and doubly occupied sites. The structure of the ground state is studied by considering the probability amplitude of intersite hopping. The results indicate that the ground state of the Mott insulator is characterized by a local antiferromagnetic order; the electrons keep some mobility, but this mobility must be compatible with the local ordering. The vanishing of some intersite probability amplitudes at $U = U_c$ puts a constrain on the electron mobility. It is suggested that such quantities might be taken as the quantities which control the order in the insulating phase.

There are several indications that the two-dimensional Hubbard model (HM) can describe a metal-insulator transition and that some kind of order is established in the paramagnetic insulating state. However, there is no clear picture about the structure of the ground state and no indication about the existence of an order parameter. In particular, there is a difficulty to conciliate the existence of a finite value for the doubly occupancy, which implies mobility of the electrons, and the existence of some order which would imply a localization of the electrons.

In this article we study the Hubbard model by means of the composite operator method (COM) in the two-pole approximation. The main results can be so summarized: (i) a Mott-Hubbard transition does exist; (ii) a local antiferromagnetic (AF) order is present in the insulating state; (iii) a quantity which controls the order in the insulating state is individuated.

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According to the band model approximation several transition oxides should be metals. In practice one finds both metallic and insulating states, with a metal-insulator transition induced by varying the boundary conditions (pressure, temperature, compound composition). Mott [1] pointed out that for narrow bands the electrons are localized on the lattice ions and therefore the correlations among them cannot be neglected. A model to describe these correlations was proposed by Hubbard [2]. In a standard notation his Hamiltonian is given by

$$H = \sum_{ij} (t_{ij} - \mu \delta_{ij}) c^\dagger(i) c(j) + U \sum_i n_\uparrow(i) n_\downarrow(i) \quad (1)$$

where $c(i)$ and $c^\dagger(j)$ are annihilation and creation operators of electrons at site i , in the spinor notation; t_{ij} describes hopping between different sites and it is usually taken as $t_{ij} = -4t\alpha_{ij}$, where α_{ij} is the projection operator on the first neighbor sites; the U -term is the Coulomb repulsive interaction between two electrons at the same site with $n_\sigma(i) = c_\sigma^\dagger(i) c_\sigma(i)$; μ is the chemical potential.

The magnitudes of the on-site Coulomb energy U and the one-electron band width $W = 8t$ control the properties of the system. In this competition between the kinetic and the potential energy the most difficult part of the model resides and exact solutions do not exist, except in some limiting cases. In particular, an adequate description of the ground state and elementary excitations is still missing. In the case of one dimension an exact solution is available [3] which shows that there is no Mott-Hubbard transition: a gap in the density of states is present for any value of U . In higher dimensions there are several results that indicate the existence of a Mott-Hubbard transition, in the sense that at half filling there is a critical value of the Coulomb potential U_c which separates the metallic phase from the insulating phase; but no rigorous results. In Hubbard I approximation [2] and in the work by Roth [4] no transition is observed [5]. In Hubbard III approximation [6] an opening of the gap is observed for $U_c = W\sqrt{3}/2$. By using the Gutzwiller variational method [7] Brinkman and Rice [8] find $U_c = 8|\bar{\epsilon}| \approx 1.65W$, with $\bar{\epsilon}$ being the average kinetic energy per electron; the vanishing of the double occupancy D at this value induced them to propose the double occupancy as an order parameter to describe the metal-insulator transition. However, this result is based on the use of the Gutzwiller approximation, which becomes exact only for infinite dimensions [9]. For finite dimensions theoretical [10] and numerical analysis [11] show that the double occupancy tends to zero only in the limit $U \rightarrow \infty$. By using the dynamical mean-field approach, or $d \rightarrow \infty$ limit, Georges et. al. [12] find that at some critical U a gap opens abruptly in the density of states, due to the disappearance of a Kondo-like peak. A recent calculation [13] of the HM in infinite dimensions shows a continuous Mott-Hubbard transition, with a gap opening at $U_c \approx W$. The same qualitative result has been found [14] by using Quantum Monte Carlo (QMC) simulation; working at the high $T = 0.33t$ the authors observe a transition with a gap opening continuously at $U_c \approx W/2$.

In conclusion, while there are several results indicating the existence of a Mott-Hubbard transition in the 2D Hubbard model, there is no unified picture; the mechanisms that lead to the transition are different; the value of the critical interaction strength varies from $U_c \approx 0.5W$ [14] up to $U_c \approx 1.65W$ [8]. A description of the structure of the ground state in the paramagnetic insulating state is also lacking.

In the framework of the COM [15,5] the Hubbard model has been solved in the two pole approximation [16], where the operatorial basis is described by the doublet Heisenberg operator

$$\psi(i) = \begin{pmatrix} \xi(i) \\ \eta(i) \end{pmatrix} \quad (2)$$

and finite life-time effects are neglected. The fields $\xi(i) = [1 - n(i)]c(i)$ and $\eta(i) = n(i)c(i)$,

with $n(i) = c^\dagger(i)c(i)$, are the Hubbard operators [2]. In this framework the single-particle propagator is given by

$$F.T.\langle R[\psi(i)\psi^\dagger(j)] \rangle = \sum_{i=1}^2 \frac{\sigma^{(i)}(\mathbf{k})}{\omega - E_i(\mathbf{k}) + i\eta} \quad (3)$$

where $F.T.$ means Fourier transform. The expressions of the spectral functions $\sigma^{(i)}(\mathbf{k})$ and energy spectra $E_i(\mathbf{k})$ have been reported in previous works [15]. These functions are calculated in a fully self-consistent treatment, where attention is paid to the conservation of relevant symmetries [15,5,17]. Differently from other approaches, one does not need to recur to different schemes in order to describe the weak- and strong-coupling regimes. *Both the limits $U \rightarrow 0$ and $U \rightarrow \infty$ are recovered by Eq. (3).*

The result (3) has been derived by assuming a paramagnetic phase. It is an open question if this is the true ground state at half filling and zero temperature. Results of numerical simulation seem to indicate that the paramagnetic phase is unstable against a long range antiferromagnetic order. However, numerical analysis is severely restricted in cluster size, and it is very hard to conclude that the true solution has an infinite range AF order. As it will be shown later, the calculation of the probability amplitudes for electron transfers shows that in the paramagnetic insulating state a local AF order is established, with a correlation length of the order of few hundred time the lattice constant.

At first, we observe that the Mott-Hubbard transition can be studied by looking at the chemical potential, which is the quantity which mostly controls the single-particle properties. Let us define

$$-\mu_1 = \left(\frac{\partial \mu}{\partial n} \right)_{n=1} = \frac{1}{\kappa(1)} \quad (4)$$

where $\kappa(n) = (\partial n / \partial \mu) / n^2$ is the compressibility. Analytical calculations show that at zero temperature there is a critical value of the interaction, fixed by the equation

$$U_c = 8t\sqrt{4p-1} \quad (5)$$

such that for $U > U_c$ the quantity μ_1 diverges. The parameter p describes a bandwidth renormalization and is defined by

$$p \equiv \frac{1}{4} \langle n_\mu^\alpha(i) n_\mu(i) \rangle - \langle [c_\uparrow(i) c_\downarrow(i)]^\alpha c_\downarrow^\dagger(i) c_\uparrow^\dagger(i) \rangle \quad (6)$$

where $n_\mu(i) = c^\dagger(i)\sigma_\mu c(i)$ is the charge ($\mu = 0$) and spin ($\mu = 1, 2, 3$) density operator. We use the notation $A^\alpha(i) = \sum_j \alpha_{ij} A(j)$ to indicate the operator A on the first neighbor site of i . The quantities p and μ_1 are functions of the external parameters n , T , U and are self-consistently calculated. Numerical solution of the self-consistent equation (5) shows $U_c \approx 1.68W$. In Fig. 1a μ_1 is plotted versus U/t for $k_B T/t = 0, 0.3, 1$. At finite temperature $-\mu_1$ increases by increasing U and tends to ∞ in the limit $U \rightarrow \infty$. At zero temperature μ_1 exhibits a discontinuity at $U = U_c$. When the intensity of the local interaction exceeds the critical value U_c , the chemical potential exhibits a discontinuity at half filling, showing the opening of a gap in the density of states and therefore a phase transition from the metallic to the insulating phase. Calculations show that the density of states (DOS) is made up by two bands: lower and upper band. When $U < U_c$ the two band overlap: metallic phase. The region of overlapping is given by $\Delta\omega = 16tp - \sqrt{U^2 + 64t^2(2p-1)^2}$. When $U > U_c$ the two band do not overlap: insulating phase. In Fig. 1b the electronic DOS is reported for different values of U . We see that when U increases the central peak opens in two peaks; some of the central weight

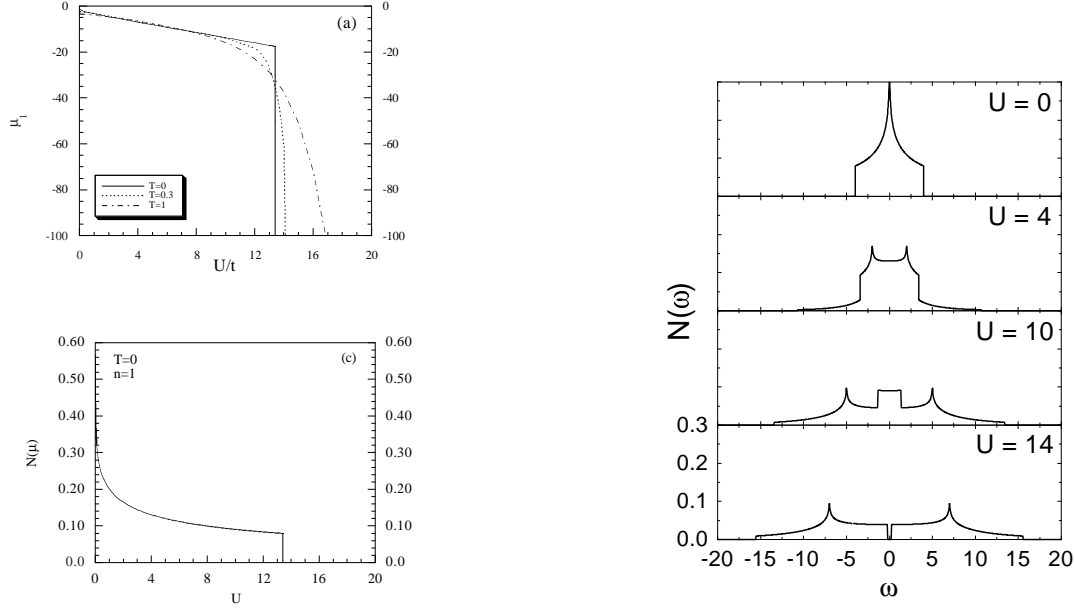


Fig. 1. – (a) The parameter $\mu_1 = -(\partial\mu/\partial n)_{n=1}$ is plotted as a function of the potential strength U/t for various values of the reduced temperature $k_B T/t$; (b) The electronic density of states at the Fermi value is given against the potential strength; (c) The electronic density of states is plotted as a function of the energy for half filling and different values of U . U/t .

is transferred to the two peaks, which correspond to the elementary excitations, described by the fields ξ and η . When U reaches the critical value $U_c \approx 1.68W$ the central peak vanishes abruptly; a gap appears and the electronic density of states splits into two separate bands. This is seen in Fig. 1c, where the DOS calculated at the Fermi level is plotted versus U . We find that the gap develops continuously, following the law $\Delta \approx 1.5W(U/U_c - 1)$.

A more detailed study of the density of states can be obtained by considering the contributions of the different channels. Calculations show that both the fields ξ and η contribute to the two bands. Only in the limit $U \rightarrow \infty$ the two operators do not interact and separately contribute to the two bands. Although, the lower band is essentially made up by the contribution of “ ξ -electron”, there is always a contribution coming from the “ η -electron”. The viceversa is true for the upper band. Particularly, the cross contribution plays an important role in the region around the Fermi value, where $N_{\xi\eta}(\mu) \approx N_{\eta\xi}(\mu) \approx N_{\eta\eta}(\mu)$ [for $U > 0$].

This result shows that in the insulating phase the ground state has a structure different from the simple one where all sites are singly occupied; the competition between the itinerant and local terms leads to a ground state characterized by a small fraction of empty and doubly occupied sites. Some questions arise: (1) what is the structure of the ground state? and in particular there exists any order?; (2) if an ordered state is established, why this order is not destroyed by the mobility of the electrons; (3) can we individuate an order parameter describing the transition at $U = U_c$? An important quantity for the comprehension of the properties of the system is the double occupancy $D = \langle n_\uparrow n_\downarrow \rangle$ which gives the average number of sites occupied by two electrons. Analytical calculations show that at zero temperature the double occupancy, as a function of U , exhibits a drastic change when the critical value is

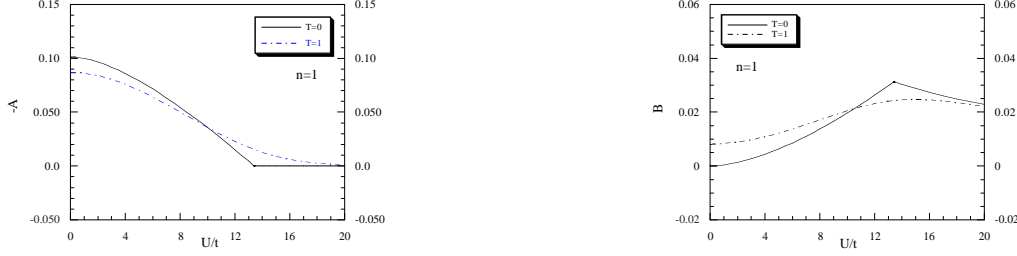


Fig. 2. – (left) The first nearest neighboring hopping amplitude $A^\alpha = \langle \xi^\alpha(i) \xi^\dagger(i) \rangle = \langle \eta^\alpha(i) \eta^\dagger(i) \rangle$ is reported as a function of U/t for zero temperature and for $k_B T/t = 1$. (right) The first nearest neighboring hopping amplitude $B^\alpha = \langle \eta^\alpha(i) \xi^\dagger(i) \rangle = \langle \xi^\alpha(i) \eta^\dagger(i) \rangle$ is reported as a function of U/t for zero temperature and for $k_B T/t = 1$.

crossed, however remains finite for $U > U_c$ and tends to zero only in the limit of infinite U as $\lim_{U \rightarrow \infty} D = J/8U$ where $J = 4t^2/U$ is the AF exchange constant. In the case of one dimension our analytical results give $\lim_{U \rightarrow \infty} D = 3t^2/U^2$ which is very close to the Bethe Ansatz result $\lim_{U \rightarrow \infty} D = 4 \ln 2 t^2/U^2$ [18]. Double occupied sites are used by the system in order to lower its energy. As a matter of fact this is precisely the origin of the effective spin-spin interaction in the $t - J$ model [19]. To better understanding the structure of the ground state, we have to study the matrix element $\langle c_\sigma(j) c_\sigma^\dagger(i) \rangle$. This quantity represents the probability amplitude that an electron of spin σ is created at site i and an electron of spin σ is destroyed at site j . However, this quantity gives only a limited information about the occupation of the sites i and j ; there are four possible ways to realize the transition $j(\sigma) \rightarrow i(\sigma)$, and the quantity $\langle c_\sigma(j) c_\sigma^\dagger(i) \rangle$ cannot distinguish among them. By means of the decomposition $c_\sigma(i) = \xi_\sigma(i) + \eta_\sigma(i)$, the probability amplitude is written as the sum of four contributions $\langle c_\sigma(j) c_\sigma^\dagger(i) \rangle = \langle \xi_\sigma(j) \xi_\sigma^\dagger(i) \rangle + \langle \xi_\sigma(j) \eta_\sigma^\dagger(i) \rangle + \langle \eta_\sigma(j) \xi_\sigma^\dagger(i) \rangle + \langle \eta_\sigma(j) \eta_\sigma^\dagger(i) \rangle$ which correspond to the following transitions:

$$\begin{aligned}
 \langle \xi_\sigma(j) \xi_\sigma^\dagger(i) \rangle : & \quad \boxed{0}_i \quad \boxed{\sigma}_j \rightarrow \boxed{\sigma}_i \quad \boxed{0}_j \\
 \langle \xi_\sigma(j) \eta_\sigma^\dagger(i) \rangle : & \quad \boxed{-\sigma}_i \quad \boxed{\sigma}_j \rightarrow \boxed{\sigma - \sigma}_i \quad \boxed{0}_j \\
 \langle \eta_\sigma(j) \xi_\sigma^\dagger(i) \rangle : & \quad \boxed{0}_i \quad \boxed{\sigma - \sigma}_j \rightarrow \boxed{\sigma}_i \quad \boxed{-\sigma}_j \\
 \langle \eta_\sigma(j) \eta_\sigma^\dagger(i) \rangle : & \quad \boxed{-\sigma}_i \quad \boxed{\sigma - \sigma}_j \rightarrow \boxed{\sigma - \sigma}_i \quad \boxed{-\sigma}_j
 \end{aligned}$$

A study of the probability amplitudes $\langle \psi(j) \psi^\dagger(i) \rangle$ will give detailed information about the structure of the ground state. In Fig. 2a the amplitude $A = \langle \xi^\alpha(i) \xi^\dagger(i) \rangle = \langle \eta^\alpha(i) \eta^\dagger(i) \rangle$ is reported as a function of U/t for two different temperatures $k_B T/t = 0, 1$. We see that in the case of zero temperature this quantity vanishes for $U > U_c$. This can be easily seen also by analytical methods. The quantity $B = \langle \eta^\alpha(i) \xi^\dagger(i) \rangle = \langle \xi^\alpha(i) \eta^\dagger(i) \rangle$ is reported in Fig. 2b; we

see that this probability amplitude does not vanish above U_c .

Owing to this contribution, we have that for $U > U_c$ the hopping of electrons from site i to the nearest neighbor is not forbidden, although restricted by the fact that $A = 0$. The hopping amplitudes have been studied up to the third nearest neighbors, but the analysis is easily extended to any site, by symmetry considerations. The scheme that emerges from analytical and numerical calculations can be summarized in the following table.

Transitions permitted for any value of U		Transitions vanishing for $U > U_c$	
$\begin{array}{ c c } \hline -\sigma & \sigma \\ \hline i & j \\ \hline \end{array} \rightleftharpoons \begin{array}{ c c } \hline \sigma & -\sigma \\ \hline i & j \\ \hline \end{array}$		$\begin{array}{ c c } \hline 0 & \sigma \\ \hline i & j \\ \hline \end{array} \rightarrow \begin{array}{ c c } \hline \sigma & 0 \\ \hline i & j \\ \hline \end{array}$	
$\begin{array}{ c c } \hline 0 & \sigma \\ \hline i & j \\ \hline \end{array} \rightarrow \begin{array}{ c c } \hline \sigma & 0 \\ \hline i & j \\ \hline \end{array}$		$\begin{array}{ c c } \hline -\sigma & \sigma \\ \hline i & j \\ \hline \end{array} \rightarrow \begin{array}{ c c } \hline \sigma & -\sigma \\ \hline i & j \\ \hline \end{array}$	
$\begin{array}{ c c } \hline -\sigma & \sigma \\ \hline i & j \\ \hline \end{array} \rightarrow \begin{array}{ c c } \hline \sigma & -\sigma \\ \hline i & j \\ \hline \end{array}$		$\begin{array}{ c c c c } \hline 0 & & & \sigma \\ \hline i & & & j \\ \hline \end{array} \rightarrow \begin{array}{ c c c c } \hline \sigma & & & 0 \\ \hline i & & & j \\ \hline \end{array}$	
$\begin{array}{ c c c c } \hline -\sigma & & & \sigma \\ \hline i & & & j \\ \hline \end{array} \rightleftharpoons \begin{array}{ c c c c } \hline \sigma & -\sigma & & 0 \\ \hline i & & & j \\ \hline \end{array}$		$\begin{array}{ c c c c } \hline -\sigma & & & \sigma \\ \hline i & & & j \\ \hline \end{array} \rightarrow \begin{array}{ c c c c } \hline \sigma & -\sigma & & -\sigma \\ \hline i & & & j \\ \hline \end{array}$	
Transitions forbidden for any value of U : $\begin{array}{ c c } \hline -\sigma & \sigma \\ \hline i & j \\ \hline \end{array} \rightleftharpoons \begin{array}{ c c } \hline \sigma & -\sigma \\ \hline i & j \\ \hline \end{array}$			

Putting all these results together, for $U > U_c$ the situation can be so summarized:

1. an electron σ which singly occupies a site (a) can hop on first, third,.....neighboring sites if and only if these sites are already occupied by an electron $-\sigma$; (b) can hop on second, fourth,.....neighboring sites if and only if these sites are empty;
2. an electron σ which doubly occupies a site (a) can hop on first, third,.....neighboring sites if and only if these sites are empty; (b) can hop on second, fourth,.....neighboring sites if and only if these sites are already occupied by an electron $-\sigma$.

The picture that emerges by these results is that the paramagnetic ground state in the insulating phase is characterized by a finite-range antiferromagnetic order. Due to the fact that there are empty and doubly occupied sites, the electrons have some mobility, but there are strong constraints on this mobility, such that the local antiferromagnetic order is not destroyed. This result is consistent with the fact that there is a competition between the itinerant and localizing energy terms. A study of the kinetic and potential energies as functions of U shows that for any $t \neq 0$ there is always some contribution which comes from the kinetic energy which allows the hopping among sites. Only in the limit of infinite U , the double occupancy and all transition amplitudes go to zero.

In conclusion, the two-dimensional single-band Hubbard model at half filling and zero temperature has been studied by means of the composite operator method. Analytical calculations show the existence of a critical value U_c which separates the metallic and insulating phases. As soon as U increases from zero, a depletion appears in the density of states; some weight of the central region is transferred to the lower and upper Hubbard bands. For larger values of U , DOS develops three separated structures: part of the weight remains in the center around the Fermi value and discontinuously disappears at $U = U_c$. Similar results, although based on different mechanism, have been previously obtained in Ref. [20] for the case of infinite-dimensional Hubbard model, in Ref. [21] by means of standard perturbation expansions, in Ref. [22] by Monte Carlo simulations. For $U > U_c$ a gap opens and the density of states splits into two separated structures. Our calculations show that even for $U \gg U_c$, where the lower and upper

bands are well separated, the two contributions coming from ξ and η do not separate. The ground state in the insulating phase contains always a small fraction of empty and doubly occupied sites.

This result is confirmed by the study of the matrix element $\langle c_\sigma(j)c_\sigma^\dagger(i) \rangle$, which gives the probability amplitude of hopping from the site j to the site i . When j is an odd nearest neighboring site of i , this quantity is not zero for $U > U_c$ and vanishes only for infinite U . However, when we split $c = \xi + \eta$ and analyze $\langle c_\sigma(j_{\text{odd}})c_\sigma^\dagger(i) \rangle$ in components, we find that for $U > U_c$ only the matrix elements $\langle \xi_\sigma(j_{\text{odd}})\eta_\sigma^\dagger(i) \rangle$ and $\langle \eta_\sigma(j_{\text{odd}})\xi_\sigma^\dagger(i) \rangle$ survive. The probability amplitudes $\langle \xi_\sigma(j_{\text{odd}})\xi_\sigma^\dagger(i) \rangle$ and $\langle \eta_\sigma(j_{\text{odd}})\eta_\sigma^\dagger(i) \rangle$ vanish at $U = U_c$ and remain zero for all $U > U_c$. On the other hand, the matrix element $\langle c_\sigma(j_{\text{even}})c_\sigma^\dagger(i) \rangle$ is always zero for any value of U ; the two contributions $\langle \xi_\sigma(j_{\text{even}})\xi_\sigma^\dagger(i) \rangle$ and $\langle \eta_\sigma(j_{\text{even}})\eta_\sigma^\dagger(i) \rangle$ compensating each other.

Summarizing, our calculations suggest that the ground state of the Mott insulator has the following characteristics: (1) a small fraction of sites are empty or doubly occupied; the number of these sites depend on the value of U/t and tends to zero only in the limit $U \rightarrow \infty$; (2) a local antiferromagnetic order is established; (3) the electrons keep some mobility, but this mobility must be compatible with the local AF order; (4) the matrix elements $\langle \xi_\sigma(j_{\text{odd}})\xi_\sigma^\dagger(i) \rangle$ and $\langle \eta_\sigma(j_{\text{odd}})\eta_\sigma^\dagger(i) \rangle$ might be considered as the quantities which control the order in the insulating phase.

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